

STN SEARCH TRANSCRIPT

10/681,205

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TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 SEP 01 New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS 4 OCT 28 KOREPAT now available on STN
NEWS 5 NOV 30 PHAR reloaded with additional data
NEWS 6 DEC 01 LISA now available on STN
NEWS 7 DEC 09 12 databases to be removed from STN on December 31, 2004
NEWS 8 DEC 15 MEDLINE update schedule for December 2004
NEWS 9 DEC 17 ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS 10 DEC 17 COMPUB updated; updating to resume; current-awareness alerts (SDIs) affected
NEWS 11 DEC 17 SDI/STATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS 12 DEC 17 CSERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS 13 DEC 17 THREE NEW FIRLS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN
NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED
NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and February 2005

NEWS EXPRESS OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0c(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 11:04:34 ON 10 JAN 2005

>> FILE REG
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
0.21 0.21
FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 11:04:41 ON 10 JAN 2005
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STRUCTURE FILE UPDATES: 7 JAN 2005 HIGHEST RN 810025-80-0
DICTIONARY FILE UPDATES: 7 JAN 2005 HIGHEST RN 810025-80-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 31, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

>>

Uploading C:\Program Files\Scinexp\Queries\HASTE SULFONYL DERIVATIVES.str



chain nodes :

7 8 9 10 11 12 13

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 4-11 7-8 7-9 7-10 11-12 11-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 1-7 2-3 3-4 4-5 4-11 5-6 7-8 7-9 7-10 11-12 11-13

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom

11:CLASS 12:Atom 13:CLASS

Generic attributes :

10:

Saturation : Unsaturated

Type of Ring System : Polycyclic

12:

Saturation : Unsaturated

Type of Ring System : Polycyclic

L1 STRUCTURE UPLOADED

>> D L1
L1 HAS NO ANSWERS
L1 STR

Structure attributes must be viewed using STN Express query preparation.

>> S L1
SAMPLE SEARCH INITIATED 11:05:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 623 TO ITERATE

100.0% PROCESSED 623 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 10963 TO 13957

PROJECTED ANSWERS: 9 TO 360

L2 9 SEA SSS SAM L1

>> FILE CAPLUS
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
0.43 0.64
FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:05:16 ON 10 JAN 2005
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FILE COVERS 1907 - 10 Jan 2005 VOL 142 ISS 3

FILE LAST UPDATED: 9 Jan 2005 (20050109/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

>> S L2
L2

>> D 1-2

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001-769282 CAPLUS

DN 135:313616

TI Heterocyclic sulfonyl compounds and activated blood coagulation factor X

(FKA) inhibitors containing them
Kobayashi, Shozo; Konoritani, Satoshi; Hagiwara, Noriyasu; Suzuki, Masanori; Yoshino, Toshiharu; Nagahara, Takayasu; Yoshikawa, Kenji; Muto, Akira; Ozanai, Takeshi; Nakamoto, Yumi; Mochizuki, Akiyoshi; Nagata, Tsutomu; Jpn. Kokai Tokkyo Koho, 304 PP.

PA Daichi Seiyaku Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 304 PP.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI JP 2001294572 A2 20011023 JP 2000-38100 20000209

PRAI JP 2000-38100 20000209

OS MARPAT 135:313616

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000-133658 CAPLUS

DN 132-194391

TI Preparation of sulfonyl moiety-containing heterocyclic compounds as factor Xa inhibitors

IN Kobayashi, Syozo; Komoriya, Satoshi; Hagiwara, Noriyasu; Suzuki, Masanori; Yoshino, Toshiharu; Nagahara, Takayasu; Nagata, Tsutomu; Horino, Haruhiko; Ito, Masayuki; Mochizuki, Akiyoshi

PA Daichi Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 883 pp.

CODEN: PIXX2D

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2000009480 A1 20000224 WO 1999-JP4344 19990811

W: AE, AL, AM, AT, AU, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KR, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MM, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KS, LS, MM, SD, SL, SZ, UG, ZW, AT, BB, CH, CY, DB, DK, ES, FI, FR, GB, GR, IS, LT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GM, ML, MR, NE, SN, TD, TG

JP 2000112953 A2 20000425 JP 1999-226878 19990810

CA 2340100 AA 20000224 CA 1999-2340100 19990811

AU 9951963 A1 20000306 AU 1999-51963 19990811

EP 1104754 A1 20010606 EP 1999-937024 19990811

R: AT, BE, BG, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

JP 2000143623 A2 20000526 JP 1999-242814 19990810

US 6747023 B1 20040608 US 2001-162888 20010212

US 2004082611 A1 20040429 US 2003-681205 20031009

PRAI JP 1998-227449 A 19980811

JP 1998-244175 A 19980828

JP 1998-251674 A 19980904

WO 1999-JP4344 W 19990811

US 2001-762888 A3 20010212

OS MARPAT 132-194391

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

APPENDIX

FULL ESTIMATED COST

2.65 3.29

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STRUCTURE FILE UPDATES: 7 JAN 2005 HIGHEST RN 810025-80-0
DICTIONARY FILE UPDATES: 7 JAN 2005 HIGHEST RN 810025-80-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryse.html>

>> S LS SSS FULL
FULL SEARCH INITIATED 11:05:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 13332 TO ITERATE

100.0% PROCESSED 13332 ITERATIONS

238 ANSWERS

SEARCH TIME: 00.00.01

L4 238 SEA SSS FUL L1

>> FILE CAPLUS
COST IN U.S. DOLLARS

SINCE FILE
ENTRY TOTAL
161.33 164.62

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:06:09 ON 10 JAN 2005
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FILE COVERS 1907 - 10 Jan 2005 VOL 142 ISS 3

FILE LAST UPDATED: 9 Jan 2005 (20050109/ED)

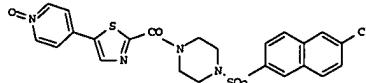
This file contains CAS Registry Numbers for easy and accurate
substance identification.

>> S L4
L5 11 L4

>> S LS NOT L3
L6 9 LS NOT L3

>> D 1-9 IB1B ABS HITSTR

L6 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004-819171 CAPLUS
DOCUMENT NUMBER: 141:374426
TITLE: Design, synthesis, and biological activity of
non-amidine factor Xa inhibitors containing pyridine
N-oxide and 2-carbamoylthiazole units
AUTHOR(S): Hagiwara, Noriyasu; Kobayashi, Syozo; Komoriya,
Satoshi; Yoshino, Toshiharu; Nagata, Tatsomi;
Hirakawa, Yumiko; Nagahara, Takayasu;
CORPORATE SOURCE: Medicinal Chemistry Research Laboratory, Daiichi
Pharmaceutical Co. Ltd, Edogawa-ku, Tokyo, 134-8630,
Japan
SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(21),
5579-5586
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB A series of thiazol-5-ylpyridine derivs. containing pyridine N-oxide and 2-carbamoylthiazole units was synthesized to optimize the S4 binding element on factor Xa. N-Oxidation of thiazol-5-ylpyridine increased the anti-fXa activity more than 40-fold independent on the position of N-oxide. The 5-pyridine N-oxide derivs. called I, were more potent than the 4-pyridine N-oxide in the presence of 1-Methylpyridine N-oxide exhibited 49-fold selectivity over thrombin. Our modeling study proposed a binding mode that the pyridine N-oxide ring of I stuck into the cation hole, and the oxide anion of I occupied in the almost same space to that of FX673. From observations of the SAR and modeling studies, we suggested the possibilities that the formation of hydrogen bond with the oxide anion in the cation hole and the affinity of cationic pyridine ring to S4 subsite were responsible for increase in anti-fXa activity.

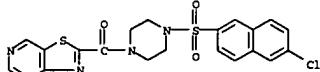
IT 222985-55-9P 259806-05-8P 782501-36-4P

782501-39-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PRSP (Preparation); USES
(Uses)

(factor Xa inhibitors containing pyridine oxide and carbamoylthiazole
units)

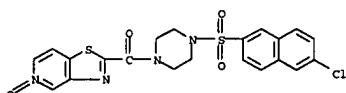
RN 222985-55-9 CAPLUS

CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-(thiazolo[5,4-c]pyridin-2-yl)carbonyl-, monohydrochloride (9CI) (CA INDEX NAME)

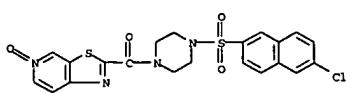


● HCl

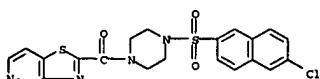
RN 259806-05-8 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(5-oxidothiazolo[4,5-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



RN 782501-36-4 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(5-oxidothiazolo[4,5-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



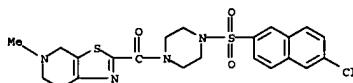
RN 782501-39-7 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-(thiazolo[4,5-c]pyridin-2-ylcarbonyl)-, hydrochloride (2:1) (9CI) (CA INDEX NAME)



● 1/2 HCl

IT 7824706-32-5 CAPLUS
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(factor Xa inhibitors containing pyridine oxide and carbamoylthiazole
units)

RN 724706-32-5 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RS FORMAT

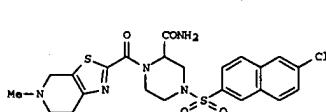
L6 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004-747454 CAPLUS

DOCUMENT NUMBER: 141:395464
TITLE: Synthesis and Conformational Analysis of a Non-Amidine Factor Xa Inhibitor That Incorporates 5-Methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine as S4 Binding Element

AUTHOR(S): Hagiwara, Noriyasu; Kobayashi, Syozo; Komoriya, Satoshi; Yoshino, Toshiharu; Suzuki, Makoto; Shimada, Takashi; Watanabe, Kengo; Hirakawa, Yumiko; Furugori, Taketoshi; Nagahara, Takayasu

CORPORATE SOURCE: Medicinal Chemistry Research Laboratory, Daiichi Pharmaceutical Co. Ltd, Edogawa-ku, Tokyo, 134-8630, Japan

SOURCE: Journal of Medicinal Chemistry (2004), 47(21), 5161-5162
PUBLISHER: JNCIAR; ISSN: 0022-2623
DOCUMENT TYPE: American Chemical Society
LANGUAGE: Journal
GI

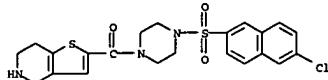


AB Our exploratory study was based on the concept that a non-amidine factor Xa (fXa) inhibitor is suitable for an orally available anticoagulant. We synthesized and evaluated a series of N-(6-chloronaphthalen-2-yl)sulfonylpiperazine derivs. incorporating various fused-bicyclic rings containing an aliphatic amine expected to be S4 binding element. Among this series, 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine type I displayed orally potent anti-fXa activity and evident prolongation of prothrombin time (PT) with the moderate bioavailability in rats. The X-ray crystal anal. afforded an obvious binding mode that 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine and 6-chloronaphthalene resp. bound to S4 and S1 subsites. In this X-ray study, we discovered a novel amide, S-O close contact. Ab initio energy calcns. of model compds. deduced that conformers with the most close S-O proximity were most stable. The Mulliken population anal. proposed that this energy profile was caused by both of electrostatic S-O affinity and N-O

repulsion. The results of these calcs. and X-ray anal. suggested a possibility that the restricted conformation effected the affinity to S4 subsite of FXa.

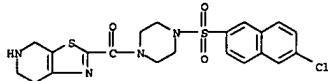
IT 222985-57-1P 222985-68-4P 222986-13-2P
 259805-64-6P 259805-66-8P 790254-92-9P
 RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, factor Xa inhibition activity and structure-activity relationship of (chlorophthalenylsulfonyl)piperazines bearing fused-heterocyclic rings)

CN 222985-57-1 CAPLUS
 Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



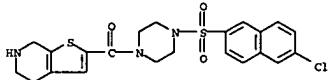
● HCl

RN 222985-68-4 CAPLUS
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● HCl

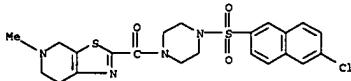
RN 222986-13-2 CAPLUS
 CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(1,2,3,4-tetrahydro-6-isoquinolinyl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

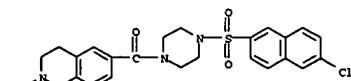
IT 222985-75-3P 222986-14-3P 259805-67-9P
 259805-88-7P 790254-66-2P 790254-72-7P
 790254-77-2P 790254-94-1P
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation, factor Xa inhibition activity and structure-activity relationship of (chlorophthalenylsulfonyl)piperazines bearing fused-heterocyclic rings)

RN 222985-75-3 CAPLUS
 CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



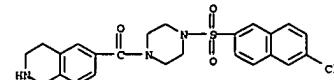
● HCl

RN 222986-14-3 CAPLUS
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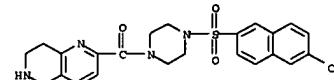
● HCl

RN 259805-67-9 CAPLUS
 CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methyl-1H-pyrido[3,2-c]pyridin-2-yl)carbonyl]-, hydrochloride (10:13) (9CI) (CA INDEX NAME)



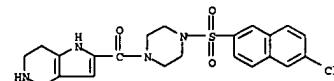
● HCl

RN 259805-64-6 CAPLUS
 CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7,8-tetrahydro-1,6-naphthyridin-2-yl)carbonyl]-, hydrochloride (10:19) (9CI) (CA INDEX NAME)



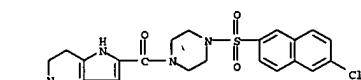
● 19/10 HCl

RN 259805-66-8 CAPLUS
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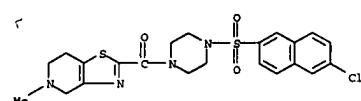
● 11/10 HCl

RN 790254-82-9 CAPLUS
 CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



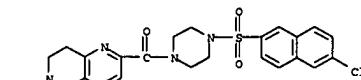
● 13/10 HCl

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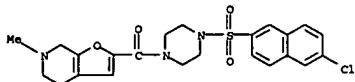
● HCl

RN 790254-66-9 CAPLUS
 CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(5,6,7,8-tetrahydro-6-methyl-1,6-naphthyridin-2-yl)carbonyl]-, hydrochloride (5:9) (9CI) (CA INDEX NAME)



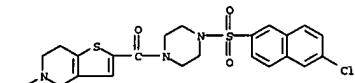
● 9/5 HCl

RN 790254-72-7 CAPLUS
 CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-6-methylfuro[2,3-c]pyridin-2-yl)carbonyl]-, hydrochloride (10:11) (9CI) (CA INDEX NAME)



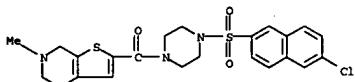
●11/10 HCl

RN 790254-77-2 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthieno[3,2-c]pyridin-2-yl)carbonyl]-, hydrochloride (5:6) (9CI) (CA INDEX NAME)



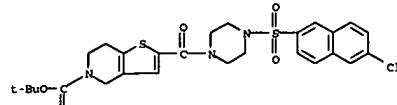
●6/5 HCl

RN 790254-84-1 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

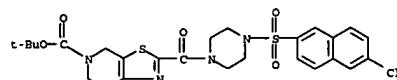


● HCl

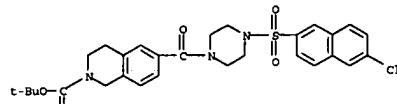
IT 222987-38-4P 222987-43-1P 222987-61-3P
259809-48-8P 259809-55-7P 790254-80-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, factor Xa inhibition activity and structure-activity relationship of (chloronaphthalenylsulfonyl)piperazines bearing fused-heterocyclic rings)
RN 222987-38-4 CAPLUS
CN Thieno[3,2-c]pyridine-5(4H)-carboxylic acid, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



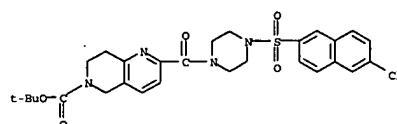
RN 222987-43-1 CAPLUS
CN Thieno[3,2-c]pyridine-5(4H)-carboxylic acid, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



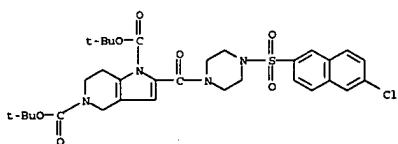
RN 222987-61-3 CAPLUS
2(1H)-Isoquinolinecarboxylic acid, 6-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-3,4-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



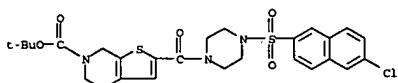
RN 259809-48-8 CAPLUS
1,6-Naphthyridine-6(SH)-carboxylic acid, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-7,8-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 259809-55-7 CAPLUS
1H-Pyrrolo[3,2-c]pyridine-1,5(4H)-dicarboxylic acid, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-6,7-dihydro-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 790254-80-7 CAPLUS
Thieno[2,3-c]pyridine-6(5H)-carboxylic acid, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-4,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS ON STN
NUMBER: 2004:362590 CAPLUS

DOCUMENT NUMBER: 141:123587

TITLE: Orally active factor Xa inhibitors:

AUTHOR(S): 4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine derivatives
Haginoya, Noriyasu; Kobayashi, Syozo; Komoriya, Satsuo; Hirokawa, Yumiko; Furugori, Taketoshi;

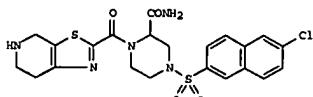
CORPORATE SOURCE: Nagahara, Takayasu
Medicinal Chemistry Research Laboratory, Daiichi Pharmaceutical Co. Ltd., Edogawa-ku, Tokyo, 134-8630, Japan

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(11), 2935-2939

PUBLISHER: CODEN: BMCLB2; ISSN: 0960-894X
DOCUMENT TYPE: Elsevier Science B.V.

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:123587
GI

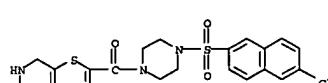


I

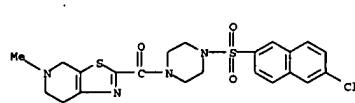
AB In an investigation of factor Xa inhibitors, a series of 1-(6-chloronaphthalen-2-yl)sulfonyl-4-(4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine-2-carbonyl)piperazines were synthesized. In vitro inhibitory activities of the compounds against factor Xa and coagulation are summarized. Among these, 4-((6-chloro-2-naphthalenyl)sulfonyl)-1-((4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl)-2-piperazinecarboxamide (I) and 4-((6-chloro-2-naphthalenyl)sulfonyl)-N-methyl-1-((4,5,6,7-tetrahydro-5-methyloxazolo[5,4-c]pyridin-2-yl)carbonyl)-2-piperazinecarboxamide, possessing a carbamoyl or N-methylcarbamoyl moiety, showed potent inhibitory activities when administered orally to rats.

IT 724706-31-4P 724706-32-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of ((chloronaphthalenyl)sulfonyl)[(tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]piperazine and study of its activity as orally active factor Xa inhibitor)

RN 724706-31-4 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

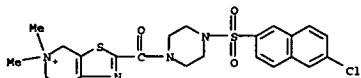


RN 724706-32-5 CAPLUS
Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthieno[3,2-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



IT 222985-77-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of [(1-chloronaphthalenyl)sulfonyl]piperazinylcarbonyltetrahydrothiazolo[5,4-c]pyridinium iodide and study of its activity as orally active factor Xa inhibitor)

RN 222985-77-5 CAPLUS
Thiazolo[5,4-c]pyridinium, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-4,5,6,7-tetrahydro-5,5-dimethyl-, iodide (9CI) (CA INDEX NAME)



● I -

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:353141 CAPLUS

DOCUMENT NUMBER: 140:357508

TITLE: Novel phosphonic acid compounds as inhibitors of serine proteases
INVENTOR(S): Greco, Michael N.; Almond, Harold R.; De Garavilla, Lawrence; Hawkins, Michael J.; Humora, Michael J.; Qian, Yun; Walker, Donald Gilmore; Cesco-Cancian, Sergio; Nilsen, Christopher Norman; Patel, Mitul N.; Sorgi, Kirk Leonard; Powell, Eugene

PATENT ASSIGNEE(S): US
SOURCE: U.S. Pat. Appl. Publ., 49 pp., Cont.-in-part of U.S. Pat. Appl. 2003 195,172.

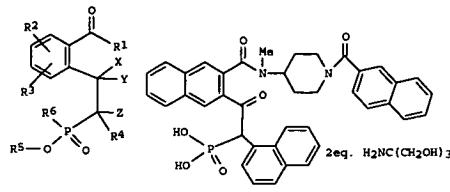
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004082544	A1	20040429	US 2003-414782	20030416
US 2003195172	A1	20031016	US 2002-273208	20021017
WO 2004094441	A2	20041104	WO 2004-US11490	20040414
W: AB, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EB, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LA, LK, LS, LT, LV, MD, ME, MG, MN, MR, MW, NG, NL, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, BY, KG, KZ, MD, RU, TJ, TN, AT, BE, BG, CH, CY, CZ, DE, DK, ES, ES, FI, FR, GB, GR, HU, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:		US 2001-330343P	P 20011019	
		US 2002-273208	B2 20021017	
		US 2003-414782	A 20030416	

OTHER SOURCE(S): MARPAT 140:357508

GI



I

II

AB The present invention is directed to phosphonic acid compds. I (R1 = amido attached heterocyclic ring, etc.; R2, R3 = substituted aromatic ring, etc.; R4 = Cl-4 alkyl, aryl, heteroaryl, cyano, halo, (halo)-1-3(Cl-8)alkyl; R5 = H, terminal carbon substituted Cl-8 alkyl, etc.; R6 = Cl-8 alkyl, aryl(Cl-8)alkyl, Cl-8 alkoxy, aryl(Cl-8)alkoxy, C2-8 alkyl, OH; X = independently selected from H, terminal carbon substituted Cl-8 alkyl, Cl-8 alkoxy, Cl-8 alkenyl, aryl(C2-8)alkenyl, aryl, aryl, aryl, OH; Y = independently selected from H, terminal carbon substituted Cl-8 alkyl, Cl-8 alkoxy, Cl-8 alkenyl, etc.) useful as serine protease inhibitors, compds. thereof and methods for treating inflammatory and serine protease mediated disorders. Thus, preparation of phosphonic acid II was described in several steps starting from di-Et 1-naphthylphosphonate and 2,3-naphthalenedicarboxylic anhydride.

IT 682356-68-7P 682356-74-7P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

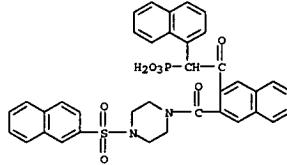
(preparation of novel phosphonic acid compds. as inhibitors of serine

proteases)

RN 682356-68-9 CAPLUS

CN Phosphonic acid, [1-(1-naphthalenyl)-2-[3-[[4-(2-naphthalenylsulfonyl)-1-

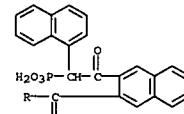
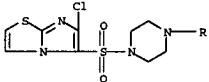
piperazinyl]carbonyl]-2-naphthalenyl]-1-(1-naphthalenyl)-2-oxoethyl] (9CI) (CA INDEX NAME)



RN 682356-74-7 CAPLUS

CN Phosphonic acid, [2-[3-[[4-((6-chloroimido[2,1-b]thiazol-5-yl)sulfonyl)-1-piperazinyl]carbonyl]-2-naphthalenyl]-1-(1-naphthalenyl)-2-oxoethyl] (9CI) (CA INDEX NAME)

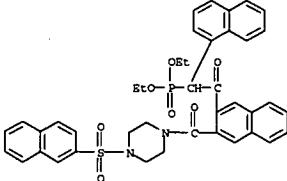
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002053579	A2	20020219	JP 2000-243754	20000811
PRIORITY APPLN. INFO.:			JP 2000-243754	20000811
OTHER SOURCE(S):			CASREACT 136:167364; MARPAT 136:167364	
GI				



IT 682356-81-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel phosphonic acid compds. as inhibitors of serine proteases)

RN 682356-81-6 CAPLUS

CN Phosphonic acid, [1-(1-naphthalenyl)-2-[3-[[4-(2-naphthalenylsulfonyl)-1-piperazinyl]carbonyl]-2-naphthalenyl]-1-(1-naphthalenyl)-2-oxoethyl] (9CI) (CA INDEX NAME)



L6 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:126365 CAPLUS

DOCUMENT NUMBER: 136:167364

TITLE: Preparation of thienopyridines as intermediates for inhibitors of activated blood coagulation factor X from pyridines

INVENTOR(S): Suzuki, Norio; Yoshioka, Toshiyuki
DAICHI Seiyaku Co., Ltd., Japan

PATENT ASSIGNEE(S): Jpn. Kokai Tokkyo Koho, 7 pp.

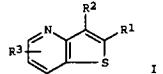
SOURCE: CODEN: JKOKAP

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:



I

AB Thienopyridines I (R1 = H, lower alkoxycarbonyl, CO2H; R2, R3 = lower alkyl) are prepared by cyclocondensation of pyridines II (R2, R3 = same as above; X = halo) with lower alkyl thioglycolate, followed by optional hydrolysis and decarboxylation. Thus, refluxing 3-fluoro-2-formylpyridine with Et thioglycolate and K2CO3 in EtOH for 1 h gave 74% I (R1 = CO2Et, R2 = R3 = H), which was hydrolyzed, converted into Li salt, amidated with 1-[(5-chloroindol-2-yl)sulfonyl]piperazine, and treated with HCl/EtOH to afford the corresponding amide HCl salt. The product inhibited activated coagulation factor X with ICS0 of 15 nM.

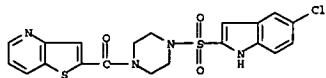
IT 368440-37-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of thienopyridines as intermediates for inhibitors of activated blood coagulation factor X from pyridines)

RN 368440-37-3 CAPLUS

CN Piperazine, 1-[(5-chloro-1H-indol-2-yl)sulfonyl]-4-(thieno[3,2-b]pyridin-2-yl)carboxylic acid, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L6 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:636077 CAPLUS
 DOCUMENT NUMBER: 135:211057
 TITLE: Preparation of N-(tetrahydrothiazolo[5,4-c]pyridin-2-ylcarbonyl)piperazine derivatives and N-(4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-ylmethyl)pyrrolidine derivative and method for inhibiting trypsin-type serine proteases
 INVENTOR(S): Komoriya, Satoshi; Hagiwara, Noriyasu; Suzuki, Makoto
 PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 234 pp.
 CODEN: PIIXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

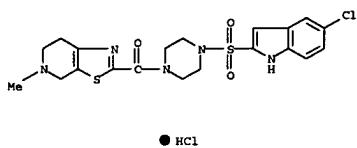
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062763	A1	20010830	WO 2001-JP1344	20010223
W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, ES, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
PRIORITY APPLN. INFO.: JP 2000-54370				A 20000225

GI

PKa: X-ray crystallog. anal. of the complexes of human G1a domain-deficient β -Pxa with the above compds. showed that bicyclic aromatic group (e.g. naphthalenyl) and aromatic heterocyclyl group (e.g. chlorindolyl) entered into the S1 pocket of the Pxa.

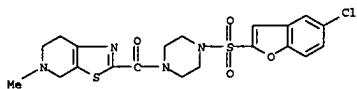
IT 259805-33-9P 357429-82-4
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of (tetrahydrothieno[3,2-c]pyridinylmethyl)piperazine derivative and method for inhibiting trypsin-type serine proteases)

RN 259805-33-9 CAPLUS
 CN Piperazine, 1-[(5-chloro-1H-indol-2-yl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 357429-82-4 CAPLUS
 CN Piperazine, 1-[(5-chloro-2-benzofuranyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:416942 CAPLUS
 DOCUMENT NUMBER: 135:19660
 TITLE: Preparation of pyrazolo[1,5-a]pyrimidines as potassium channel inhibitors
 INVENTOR(S): Atwal, Karnail S.; Vaccaro, Wayne; Lloyd, John; Finley, Heather; Yan, Lin; Bhandaru, Rao S.
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 298 pp.
 CODEN: PIIXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1

AB Trypsin-type serine protease inhibitors are compds. having groups represented by the general formula (I) or (II) (wherein R1 and R2 are each hydrogen, Cl-3 alkyl, halo, C2-3 alkenyl, or ethynyl; or R3 and R4 are each hydrogen, hydroxyl, or amino; X1, X2, X3 and X4 are each CH or N; Y1 and Y2 are each CH or N; and Y3 is NH, O or S). When such a compound is made to act on a trypsin-type serine protease, e.g. factor Xa (Fxa), the group enters the S1 pocket thereby exert an inhibitory activity against the protease. Thus, to a solution of 400 mg 1-[(5-chloroindol-2-yl)sulfonyl)piperazine in 100 mL DMF were added 1-hydroxybenzotriazole 10.5, 1-ethyl-3-(dimethylaminopropyl)carbodiimide hydrochloride 194, lithium 5-methyl-1,4,5,6,7-tetrahydrothiazolo[5,4-c]pyridinecarboxylate 175, and N-methylmorpholine 86.8 mg, and the resulting mixture was stirred at room temperature for 10 h to give 1-[(5-chloroindol-2-yl)sulfonyl]-4-(5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-ylcarbonyl)piperazine hydrochloride (III.HCl). III.HCl showed IC50 of 0.005 μ M against human

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001040231	A1	20010607	WO 2000-US32785	20001204
W: AS, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, ES, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
CA 2393809	AA	20010607	CA 2000-2393809	20001204
BP 1237891	A1	20020911	BP 2000-980930	20001204
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, IE, SI, LT, LV, FI, RO, MK				
BR 2000061656	A	20030424	BR 2000-16166	20001204
JP 2004507442	T2	20040311	JP 2001-540986	20001204
NZ 518663	A	20041126	NZ 2000-518663	20001204
US 2003022890	A1	20030130	US 2000-729731	20001205
US 6706720	B2	20040316		
ZA 2002003407	A	20030925	ZA 2002-3407	20020429
NO 2002002649	A	20020606	NO 2002-2649	20020605
US 2004063687	A1	20040401	US 2003-660878	20030912

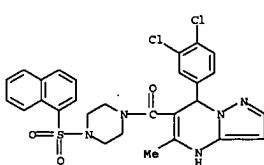
PRIORITY APPLN. INFO.: MARPAT 135:19660

GI

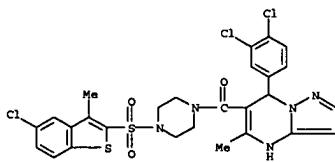
function (especially inhibitors of the Kv1 subfamily of voltage gated K+ channels, especially inhibitors Kv1.5 which has been linked to the ultrarapidly activating delayed rectifier K+ current IKur) in the prevention and treatment of arrhythmia and IKur-associated conditions, were prepared. Thus, reacting Me acetoacetate with 2,3-dichlorobenzaldehyde in the presence of piperidine and AcOH in PhMe followed by refluxing the resulting intermediate II with 3-aminopyrazole in 1-propanol afforded the title compound III. The compds. I are effective at 0.001-100 mg/kg/day.

IT 343244-51-9 343244-55-3P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of pyrazolo[1,5-a]pyrimidines as potassium channel inhibitors)

RN 343244-51-9 CAPLUS
 CN Piperazine, 1-[(7-(3,4-dichlorophenyl)-4,7-dihydro-5-methylpyrazolo[1,5-a]pyrimidin-6-yl)carbonyl]-4-(1-naphthalenylsulfonyl)- (9CI) (CA INDEX NAME)



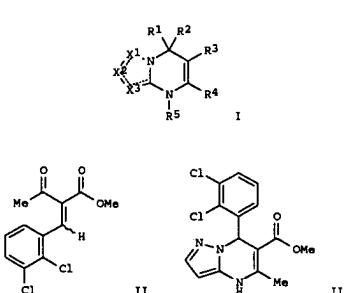
RN 343244-55-3 CAPLUS
 CN Piperazine, 1-[(5-chloro-3-methylbenzo[b]thien-2-yl)sulfonyl]-4-[(7-(3,4-dichlorophenyl)-4,7-dihydro-5-methylpyrazolo[1,5-a]pyrimidin-6-yl)carbonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:76377 CAPLUS
 DOCUMENT NUMBER: 134:131538
 TITLE: Preparation of imidazolimidazoles and triazoles as anti-inflammatory agents
 INVENTOR(S): Wu, Jiang-Ping; Kelly, Terence Alfred; Lemieux, Rene M.; Goldberg, Daniel R.; Emeigh, Jonathan Emilian; Sorcek, Ronald J.

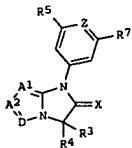
AB The title compds. [I; X1-X3 = N, NR6, (CR7)q, (CR7)q, CO; R1-R7 = (CH2)n(CH2)pZ2; or R1-R5 may, in one or more pairs of two, together with the atoms to which they are bonded, form (un)substituted carbocyclic, heterocyclic group; or R6 and R7 may, together with the atoms to which they are bonded, form (un)substituted carbocyclic, heterocyclic group; Z1 = O, S, CO, etc.; Z2 = H, NO2, halo, etc.; n, p = 0-10 (when m = 0, p is also 0); m = 0-1; q = 1-3], useful as inhibitors of potassium channel



PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 368 pp.
 CODEN: PIXDD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
 WO 2001007440 A1 20010201 WO 2000-US18884 20000712
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CZ, CH, CN, CU, CT, DE, DK, ES, FI, GB, GD, GE, GR, GM, HK, HU, ID, IL, IS, IT, JP, KE, KW, LV, LT, LU, LV, MW, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UR, US, UA, VN, ZA, ZW
 RW: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 US 6492408 B1 20021210 US 2000-604312 20000627
 CA 2383017 AA 20010201 CA 2000-2383017 20000712
 BE 2000012666 A 20020409 BE 2000-12666 20000712
 EP 1216247 A1 20020626 EP 2000-948618 20000712
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL
 TR 200200160 T2 20021021 TR 2002-200200160 20000712
 JP 200305460 T2 20030212 JP 2001-512524 20000712
 EE 20020028 A 20030415 EE 2002-28 20000712
 NZ 20020028 A 20030427 NZ 2000-517217 20000712
 AU 776496 B2 20030309 AU 2000-4091 20000712
 BG 106312 A 20020930 BG 2002-106312 20020116
 ZA 2002000428 A 20030117 ZA 2002-428 20020117
 NO 2002000275 A 20020204 NO 2002-275 20020118
 US 2003203955 A1 20031030 US 2002-195973 20020716
 US 6689804 B2 20040210 20000712
 US 2004116426 A1 20040617 US 2003-672412 20030925
 US 1999-144905P P 19990721
 US 1999-150939P P 19990826
 US 2000-604312 A1 20000627
 WO 2000-US18884 W 20000712
 US 2002-195973 A3 20020716
 PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 134:131538
 GI



AB Compds. I (A1 = N, CH; A2 = N, CH, CR'; R' = halo, cyano, alkoxy, alkoxycarbonyl, alkylsulfonyl; R = N, CH, CR1, C(S(=O)R1), C(=O)R1, C(S(=O)R1), C(=O)R1; R1, R1a = (substituted) alkyl, cycloalkyl, aryl, or heteroaryl groups, alkyl groups containing 2-6 carbons substituted with carboxylate, phenophenone, sulfonate, amidine, or

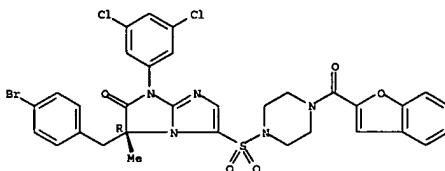
guanidine moieties, amino, halogen, cyano; R3 = H, alkyl, cycloalkyl, alkoxy or amino substituted alkyl, cycloalkyl; R4 = substituted arylmethyl; R5 = Cl, F3C, cyano, O2N, F3C; X = O, S; if Z = N or CH, R7 = Cl, F3C, cyano, O2N; Z = N, CR6 where R6 = H, halo, Me, cyano, F3C, based mostly on imidazo[1,2-a]imidazole and imidazo[1,2-a]triazole nuclei, are prepared as inhibitors of leukointegrins to cell adhesion molc. in the treatment or prevention of inflammatory and immune cell-mediated diseases. E.g., (R)-I (A1 = N; A2 = D = CH; R3 = Me; R4 = 4-Brc6H4CH2; R5 = R7 = Cl; X = O; Z = CH) (II) was prepared from (R)-a-methyl-4-bromophenylalanine Me ester and 3,5-dichlorophenylisothiocyanate by heating in 1,4-dioxane to give a thiophhydrantoin which was treated with N-(triphenylphosphoranylidene)-1,3-dioxolan-2-ylmethylamine [prepared from 2-(azidomethyl)-1,3-dioxolan-2-ylmethylamine and triphenylphosphine] to give a dihydro-1,3-dioxolan-2-ylmethylamine derivative; treatment of the intermediate with trifluoroacetic acid and heating at 90° overnight gave II with m.p. 36-37.5°. I inhibited binding of leukointegrins to cell adhesion molc. with Kd=10 μM.

IT 321723-06-27 CAPLUS
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of imidazo[1,2-a]imidazole and imidazo[1,2-a]triazole derivs. as inhibitors of leukointegrin binding to cell adhesion molc. in the treatment of inflammatory and immune-cell mediated diseases)

RN 321723-06-2 CAPLUS

CN Piperazine, 1-(2-benzofurazan-2-yl)-2,3-dihydro-3-methyl-2-oxo-1H-imidazo[1,2-a]imidazol-5-yl)sulfonyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

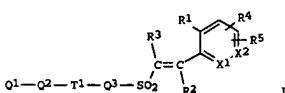


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1999-233901 CAPLUS
 130:296694
 DOCUMENT NUMBER:
 Preparation of heterocyclic compounds having the sulfonyl group as antithrombotics
 INVENTOR(S): Kobayashi, Shozo; Komoriya, Satoshi; Ito, Masyuki; Nagata, Tautomu; Mochizuki, Akiyoshi; Higino, Noriyasu; Nagahara, Takayasu; Horino, Haruhiko
 PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
 SOURCES: PCT Int. Appl., 342 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
 WO 9916747 A1 19990408 WO 1998-JP4411 19980930
 W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CZ, CH, CN, CU, CT, DE, DK, ES, FI, GB, GD, GE, GR, GM, HK, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TZ, TM, FI, FR, GB, GR, IS, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 CA 2304285 AA 19990408 CA 1998-2304285 19980930
 AU 9892806 A1 19990423 AU 1998-92806 19980930
 EP 1031563 A1 20000830 EP 1998-945542 19980930
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI
 BR 9815377 A 20010116 BR 1998-15377 19980930
 US 6525042 B1 20030225 US 2000-508680 20000324
 NO 2000001636 A 20000329 NO 2000-508680 20000324
 US 2003232809 A1 20031218 US 2002-262978 20021220
 PRIORITY APPLN. INFO.:

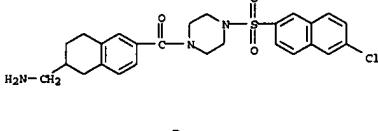
OTHER SOURCE(S): MARPAT 130:296694
 GI



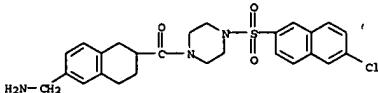
AB The title compds. I (R1 is hydrogen, hydroxyl, nitro or the like; R2 and R3 are each independently hydrogen, halogeno or the like; R4 and R5 are each independently hydrogen, halogeno or the like; Q1 is an optionally substituted saturated or unsatd. 5- or 6-membered cyclic hydrocarbon group or the like; Q2 is a single bond, oxygen or the like; Q3 is a heterocyclic moiety (represented by 4 generic structures); T1 is carbonyl or the like; and X1 and X2 are each independently methine or nitrogen) are prepared. I speedily exert satisfactory and persistent antithrombotic effects through oral administration and cause few adverse effects. I is an in vitro test for inhibition of activated blood coagulation factor X. I (1-(6-chlorophenyl)-2-(6-methyl-4,5,6,7-tetrahydrothiopheno[5,4-c]pyridin-2-yl)sulfonyl)-4-(6-methyl-4,5,6,7-tetrahydrothiopheno[5,4-c]pyridin-2-yl)carbonylpiperazine hydrochloride showed the K1 value of 6.6 nM.

IT 222985-32-222985-35-5P 222985-35-5P 222985-36-6P 222985-38-8P 222985-49-1P 222985-50-4P 222985-51-5P 222985-52-6P 222985-53-7P 222985-55-9P 222985-57-1P 222985-64-0P 222985-67-3P 222985-68-4P 222985-69-5P 222985-70-8P 222985-71-9P 222985-73-1P 222985-75-3P 222985-77-5P 222985-79-7P 222985-86-6P 222985-88-8P 222985-89-9P 222985-90-2P 222986-01-8P 222986-04-1P 222986-14-1P 222986-15-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of heterocyclic compds. having the sulfonyl group as

antithrombotics)
 RN 222985-32-2 CAPLUS
 CN Piperazine, 1-[(6-aminomethyl)-5,6,7,8-tetrahydro-2-naphthalenyl]carbonyl-4-((6-chloro-2-naphthalenyl)sulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

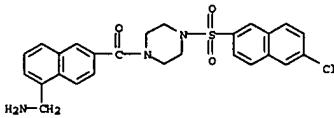


RN 222985-35-5 CAPLUS
 CN Piperazine, 1-[(6-aminomethyl)-1,2,3,4-tetrahydro-2-naphthalenyl]carbonyl-4-((6-chloro-2-naphthalenyl)sulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



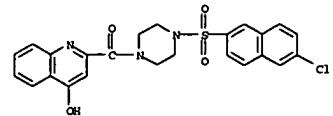
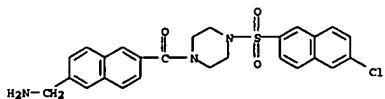
● HC1

RN 222985-36-6 CAPLUS
 CN Piperazine, 1-[(6-aminomethyl)-2-naphthalenyl]carbonyl-4-((6-chloro-2-naphthalenyl)sulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



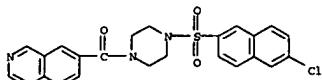
● HC1

RN 222985-38-8 CAPLUS
 CN Piperazine, 1-[(6-aminomethyl)-2-naphthalenyl]carbonyl-4-((6-chloro-2-naphthalenyl)sulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

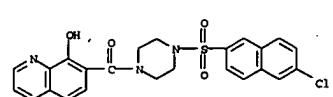


● HCl

RN 222985-49-1 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-(7-isoquinolinylcarbonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

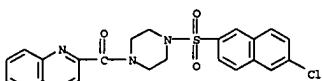


RN 222985-52-6 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(8-hydroxy-7-quinolinyl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

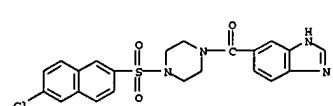


● HCl

RN 222985-50-4 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-(2-quinolinylcarbonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



RN 222985-53-7 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(6-chloro-2-naphthalenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

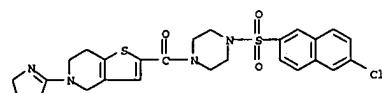
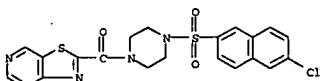


● HCl

RN 222985-51-5 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4-hydroxy-2-quinolinyl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

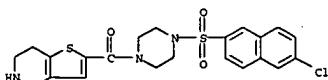
● HCl

RN 222985-55-9 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-(thiazolo[5,4-c]pyridin-2-ylcarbonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



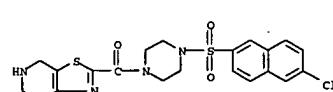
● HCl

RN 222985-57-1 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 222985-68-4 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

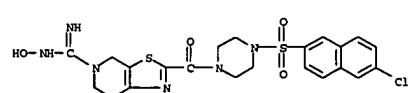


● HCl

RN 222985-64-0 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-(hydroxymino)iminomethylthieno[3,2-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 222985-69-5 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-(hydroxymino)iminomethylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

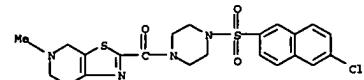
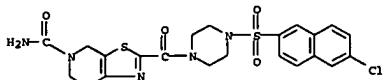


● HCl

RN 222985-67-3 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(5-(3,4-dihydro-2H-pyrol-5-yl)-4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

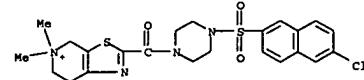
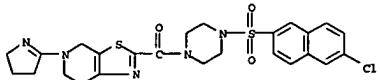
● HCl

RN 222985-70-8 CAPLUS
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxamide, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-6,7-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



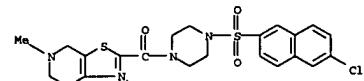
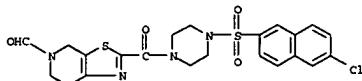
● HCl

RN 222985-71-9 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(5-(3,4-dihydro-2H-pyrrrol-5-yl)-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 222985-73-1 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(5-formyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

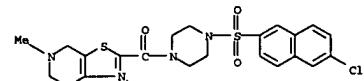


● HCl

RN 222985-75-3 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

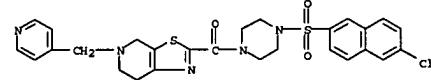
● I-

RN 222985-79-7 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methyl-1-oxidothiazolo[5,4-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



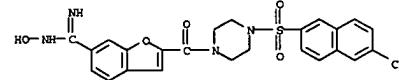
● I-

RN 222985-86-6 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-(2-hydroxyethyl)thiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



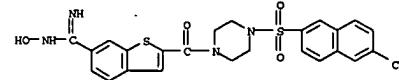
● HCl

RN 222986-01-8 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(6-(hydroxyamino)iminomethyl)-2-benzofuranyl]carbonyl-, monohydrochloride (9CI) (CA INDEX NAME)



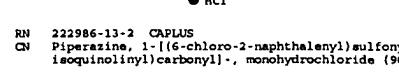
● HCl

RN 222986-04-1 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(6-(hydroxyamino)iminomethyl)benzo[b]thien-2-yl]carbonyl-, monohydrochloride (9CI) (CA INDEX NAME)

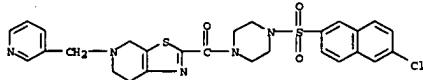


● HCl

RN 222986-13-2 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(1,2,3,4-tetrahydro-6-isooquinolinyl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

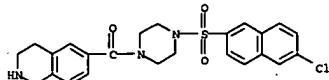


RN 222985-89-9 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-(3-pyridinylmethyl)thiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



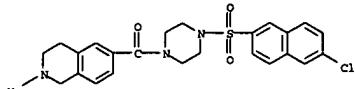
● HCl

RN 222985-90-2 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-(4-pyridinylmethyl)thiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



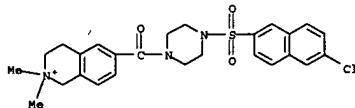
● HCl

RN 222986-14-3 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(1,2,3,4-tetrahydro-2-methyl-6-isquinolinyl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

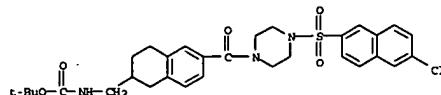
RN 222986-15-4 CAPLUS
CN Isoquinolinium, 6-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-1,2,3,4-tetrahydro-2,2-dimethyl-, iodide (9CI) (CA INDEX NAME)



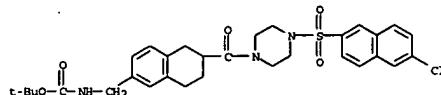
● I⁻

IT 222986-96-1P 222987-04-4P 222987-06-6P
222987-38-4P 222987-40-8P 222987-43-1P
222987-56-6P 222987-57-7P 222987-61-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic compds. having the sulfonyl group as antithrombotics)
RN 222986-96-1 CAPLUS
CN Carbamic acid, [(6-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-1,2,3,4-tetrahydro-2-naphthalenyl)methyl]-,

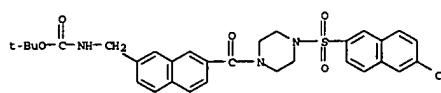
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



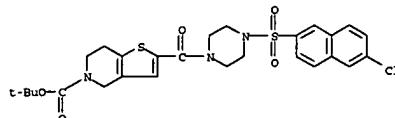
RN 222987-04-4 CAPLUS
CN Carbamic acid, [(6-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-1,2,3,4-tetrahydro-2-naphthalenyl)methyl]-1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



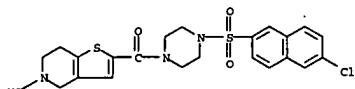
RN 222987-06-6 CAPLUS
CN Carbamic acid, [(1-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-2-naphthalenyl)methyl]-1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



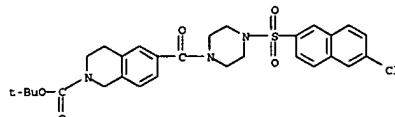
RN 222987-38-4 CAPLUS
CN Thieno[3,2-c]pyridine-5(4H)-carboxylic acid, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 222987-40-8 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(5-cyano-4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



RN 222987-43-1 CAPLUS
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> LOGOFF
ALL LW QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:N

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	45.36	209.98
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.57	-6.57

FILE 'MEDLINS' ENTERED AT 11:07:16 ON 10 JAN 2005

FILE LAST UPDATED: 8 JAN 2005 (20050108/UP). FILE COVERS 1950 TO DATE.

On December 19, 2004, the 2005 MeSH terms were loaded.

Warning: The search L-number/HUMAN limit is missing from records indexed with the new 2005 MeSH (records added since December 19, 2004). Until this is corrected, include HUMANS/CT and 20041219-20051231/ED in searches to limit results to humans for this time period.

OLDMEDLINS now back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2005 vocabulary. See <http://www.nlm.nih.gov/mesh/> and http://www.nlm.nih.gov/pubs/techbull/nd03_nd03_mesh.html for a description of changes.

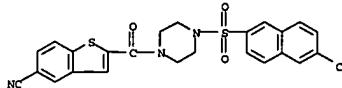
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> LOGOFF
ALL LW QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.38	210.36
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-6.57

STN INTERNATIONAL LOGOFF AT 11:07:20 ON 10 JAN 2005

RN 222987-57-7 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(5-cyanobenzo(b)thien-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



RN 222987-61-3 CAPLUS
CN 2(1H)-Isquinolincarboxylic acid, 6-[(4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl)carbonyl]-3,4-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)